

Defect Segregation Facilitates Oxygen Transport at Fluorite UO_2 Grain Boundaries

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Supporting Information

Table 1: S1 - Potential parameters for the Morl potential model. The superscripts on the species represent the charges of the atoms.

Ion Pair	D_{ij} (eV)	B_{ij} (Å)	r_0 (Å)	$A_{ij}(eVA^{12})$
$O^{1.2} - O^{1.2}$	0.041730	1.886824	3.189367	22
$U^{2.4} - O^{1.2}$	0.083352	1.946417	2.946396	1
$Fe^{1.8} - O^{1.2}$	0.029584	2.575402	2.559207	3
$Gd^{1.8} - O^{1.2}$	0.028451	2.057296	3.074956	3
$La^{1.8} - O^{1.2}$	0.070053	1.3984	3.382429	3

Table 2: S2 – Total number of atoms in each grain boundary supercell and the total number of dopants and oxygen vacancies added.

Grain Boundary	Number of Atoms	GB Width (Å)	Number of Species	
			M^{3+}	V_o
$\Sigma 3(111)$	8640	20.00	30	15
$\Sigma 11(311)$	7200	20.00	24	12
$\Sigma 5(210)$	7680	21.00	26	13
$\Sigma 5(310)$	7680	20.00	26	13
$\Sigma 9(221)$	5760	20.00	20	10
$\Sigma 19(331)$	7200	17.00	24	12

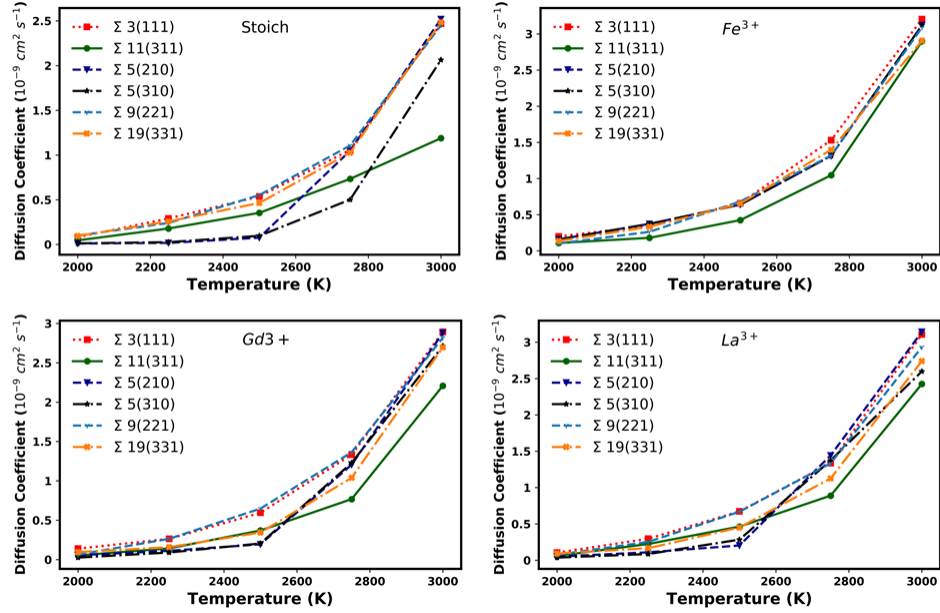


Figure 1: Diffusion Coefficients

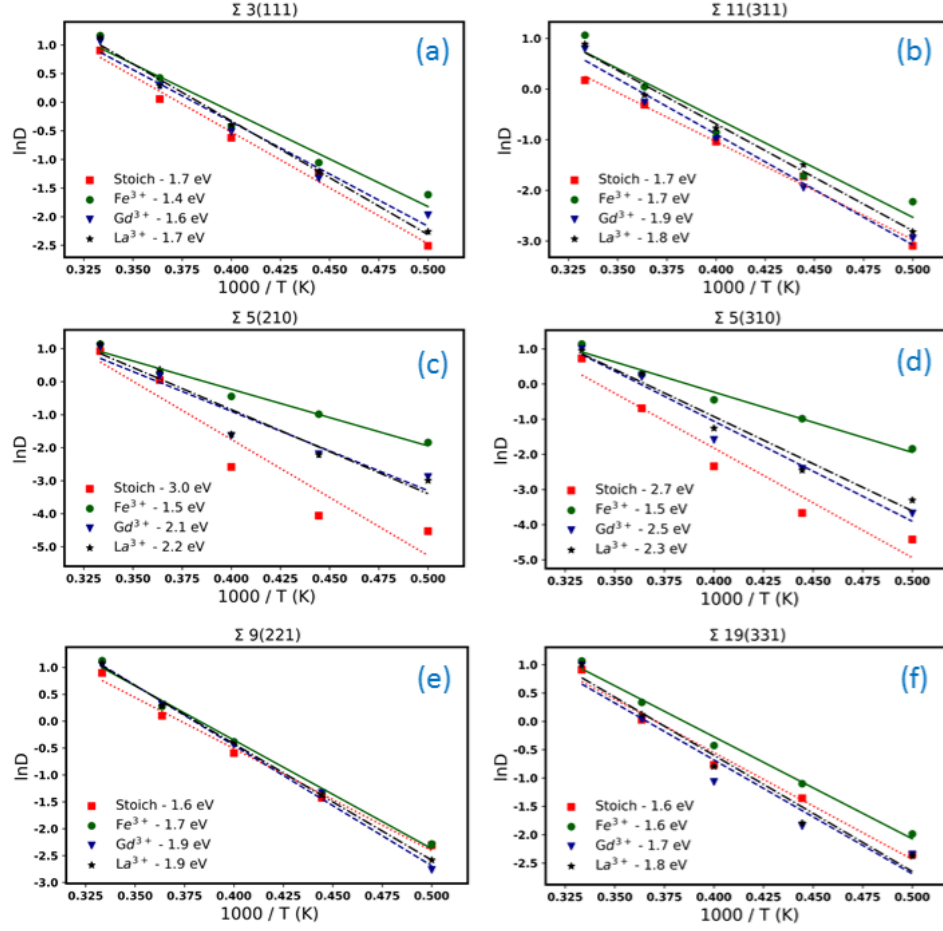


Figure 2: Arrhenius plots for oxygen in the $\Sigma 3(111)$, $\Sigma 11(311)$, $\Sigma 5(210)$, $\Sigma 5(310)$, $\Sigma 9(221)$ and $\Sigma 19(331)$ boundaries (a), (b), (c), (d), (e) and (f). Stoichiometric, Fe^{3+} doped, Gd^{3+} doped and La^{3+} doped boundaries are denoted by (red squares), (green circles), (blue triangles) and (black stars).